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Optimized calibration and measurement procedures in rotating analyzer and rotating polarizer ellipsometry

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Accurate spectroellipsometric (SE) measurements in the rotating analyzer (RAE) or rotating polarizer (RPE) configurations require accurate values of the polarizer/analyzer(/retarder) azimuths. While the readings are usually fairly accurate, true values are influenced by possible offsets between the plane of incidence, physical axes of the elements, and the instrument scales. The offsets are often determined by specialized calibration procedures. We describe SE measurements designed to obtain the calibration parameters together with the target ellipsometric spectra. We use multiple settings of the polarizer (analyzer) azimuths in RAE (RPE), respectively, to optimize precision and accuracy of SE measurements, and to economize measurement time. The optimization concerns the choice of measurement parameters as well as the subsequent data analysis. We present in detail examples of visible-ultraviolet measurements.

1. Introduction

In visible and nearby spectral bands, spectroscopy with CDD detectors offers a conveniently fast technique compared to the monochromator-based instruments. In ellipsometric applications (for one fixed and one rotating polarizing element) all Fourier coefficients are extracted at the same time throughout the spectrum. The classical calibration procedure devised by [1] is based on measurements at several polarizer (in the case of RAE) or analyzer (for RPE setup) settings centered around the (presumed) zero position. The principles for these setups and the analysis of ellipsometric data can be found in [2].

While with single-energy measurements (using a monochromator) this can be a relatively fast process; with the CCD-based detectors this calibration may take considerably longer times than the measurement itself, since the whole spectrum is collected for each polarizer setting, while the rotating element moves at a slower speed due to integration times required by the detector. The same arguments apply to the Fourier-transform technique in infrared, where the entire spectral range is recorded simultaneously with the duration of each scan typically of the order of seconds. Here we propose an alternative calibration procedure based on the measured spectra themselves, resulting in a more efficient use of the measurement time. With this approach no extra experimental effort is needed to measure the polarizer and analyzer offsets, as we derive these auxiliary quantities directly from the target spectra.

In the next section we describe the standard method of Aspnes and estimate its errors, then in Sec. 3 we present our calibration procedure together with some related methods. In Sec. 4 these two methods are applied on ellipsometric measurements of one chosen sample. Then we turn to the simulations in order to estimate reconstruction capabilities of our method: we map errors in Ψ (Sec. 5), we quantify effects of our initial estimate of the offsets (Sec. 6) and finally we check the performance of our method for a variety of synthetic spectra (Sec. 7).

2. Errors of standard calibration

In the standard calibration procedure the Fourier coefficients a_2 and b_2 are measured around the zero polarization angle P (in the following we will be considering the RAE setup only). The true position of the polarizer parallel to the plane of incidence corresponds to the minimum of the residual $1-a_2^2-b_2^2$. It can be approximated with a parabola $f(P)=c_0+P\,c_1+P^2\,c_2$, whose minimum is $P_{\min}=-c_1/(2c_2)$. The errors of the parameters c_j depend only on the positions of the measurement points P_i (and their higher moments): if these are chosen symmetrically around zero (and all odd-order moments vanish), we have $\delta c_0=N$, $\delta c_1=\sqrt{(\sum P_i^2)}$, and $\delta c_2=\sqrt{(\sum P_i^4-(\sum P_i^2)^2)}$, where N is the number of measurement points. Using these values we obtain

$$\delta^2 P_{\min}=\left(\frac{1}{2c_2}\right)^2\delta^2 c_1+\left(\frac{c_1}{2c_2^2}\right)^2\delta^2 c_2. \tag{1}$$

The correction for the null position of the analyzer is obtained from the same set of measurements, looking at the P dependence of the

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phase-angle $g(P) = 0.5\ \arctan(b_2(P)/a_2(P))$, which is almost linear in the region of interest; the error $\delta P_{\min}$ is thus propagated also into the error of $A_0 = g(P_{\min})$.

We have tested this process using the measurements of Fourier coefficients a_2 and b_2 on a real sample (the same as described in Sec. 4), in the visible for 13 polarizer positions from −6 to 6°. The whole visible spectra of 800 points were divided in 12 intervals where P_0 and A_0 were estimated independently using the average value of Fourier coefficients in the interval. The parabolic shape fitted well the dependence on P if the dataset has been limited to 7 measurements in a narrower range from −3 to 3°. The dispersion of the values of P_0 and A_0 obtained in this way corresponded well to the theoretical estimates above, $\delta P_0 = 0.05°$ and $\delta A_0 = 0.14°$.

3. Calibration using symmetrical positions of the polarizer

A minimal dataset for our alternative method consists of two measurements taken with the polarizer settings P_a and $-P_a$. If the zero position was truly at $P_0 = 0$, the Fourier coefficients a_2 would be identical (since they depend only on the absolute value of tan P) and b_2 would have an opposite sign; averaging the two spectra is equivalent to the 2-zone ellipsometric scheme [3]. In reality, the effect of a small offset P_0 on the Fourier coefficients can be estimated with the help of the derivatives

$$\frac{\partial a_2}{\partial P_0} = -\frac{2\tan^3(P_a - P_0)}{\left(\tan^2(P_a - P_0) + \tan^2\Psi\right)^2 \cos^2(P_a - P_0)}, \tag{2}$$

$$\frac{\partial b_2}{\partial P_0} = \frac{2\tan\Psi\cos\Delta\left(\tan^2(P_a - P_0) - \tan^2\Psi\right)}{\left(\tan^2(P_a - P_0) + \tan^2\Psi\right)^2 \cos^2(P_a - P_0)}. \tag{3}$$

The misalignment A_0 of the analyzer adds another rotation of the vector (a_2, b_2). P. Maršík in [4] has described a method based on a transformation in the (a_2, b_2) plane that allows to correct both analyzer and polarizer offsets (a similar idea to perform the fitting procedure in the (a_2, b_2) plane was already presented in [5]). It converts all the measurements to a single position of the polarizer. This approach has the advantage of not suffering from possible singular points in the non-linear transformation between the ellipsometric angles and Fourier coefficients: the conversion in the plane of Fourier coefficients is linear. In our method, large errors of ellipsometric angles appear in points where $\mathrm{abs}(a) \to 1$ and, esp. for Δ, also where sin Δ vanishes.

Now let us outline principal steps of our calibration method. In order to be able to use several pairs of the ellipsometric spectra at polarization settings at hand, we use the following basic idea: we convert the measurements to Ψ and Δ and look for the offsets leading to the datasets differing in these new variables as little as possible. In particular, the optimum of calibration corrections (P_0 and A_0) is estimated as that minimizing the weighted sum of dispersions at each spectroscopic point of the ellipsometric angles calculated from the measurements at different polarizer angles. For the sake of robustness, with more than three datasets available, the most deviating measurement at each spectral point is rejected from the calculation. Non-linear effects both in the CCD detector and optical elements are usually negligible; they are readily monitored by calculations of higher-order Fourier coefficients.

4. Measurements on multilayers

We illustrate the new calibration method on our recent measurements of multi-layered samples of molybdenum nanostructures in silica deposited on a silicon substrate. We have chosen the angle of incidence of 67° to match that of the VUV ellipsometer at NIM-3 beamline of BESSY-II synchrotron. The VUV spectra were calibrated at a single energy (5 eV) using the conventional method of Aspnes, while our calibration procedure was applied to the CCD measurements in the visible and near-UV. A fairly good overlap of reconstructed ellipsometric parameters in the three ranges strengthens the confidence in both methods.

Usually our measurements have been done with the polarizer set to ±20 and ±30°; in the case of the sample shown in Fig. 1 we added also a third pair at ±40°. Having found the minimum of the sum of dispersions in the (A_0, P_0) plane, we can scan its vicinity to obtain standard errors of the fitted offsets. When we combine data from several pairs of polarizer settings, the resulting map shows a much lower correlation between A_0 and P_0; on the other hand several false secondary minima can appear. For the combined calibration we find $\delta P_0 = 0.03°$ and $\delta A_0 = (+0.08/-0.22)°$, slightly better than the values obtained for the single-energy calibration.

5. Simulations and error maps

The offsets and their errors are, however, merely auxiliary quantities entering the calculations of the wanted spectra. Let us turn now to synthetic spectra that allow us to study how the errors, i.e. shifts in the (A_0, P_0) plane influence the wanted values of the ellipsometric angles Ψ and Δ.

Using the simulations we scan the mean errors of reconstructed ellipsometric angles, i.e. the difference from the input ones integrated over the whole spectrum, in the (A_0, P_0) plane, providing sensitivity maps of these physical results with respect to the uncertainty of δA_0 and δP_0. Fig. 2 shows a calibration using a single pair of $P_0 = \pm 30°$, compared to a rather complicated situation of Fig. 3 that results from the more robust estimate using 4 pairs of polarizer settings (±10°, ±20°, ±30° and ±40°). The spectrum used corresponded to a slowly rising Ψ with a mean value of 22° and $\Delta = 12°$. We see the largest improvement of the error of reconstructed Ψ in the center of the graph, corresponding to the true values of offsets, $P_0 = 2°$ and $A_0 = 2°$. The effect on the reconstruction error, almost constant (within the region of one standard error in A_0 and P_0) in the case of the single-pair calibration, becomes very irregular when combining multiple measurements.

6. Offset of the initial guess

We have further studied the dependence of the errors of the estimation of the misalignments, i.e. the difference between calculated

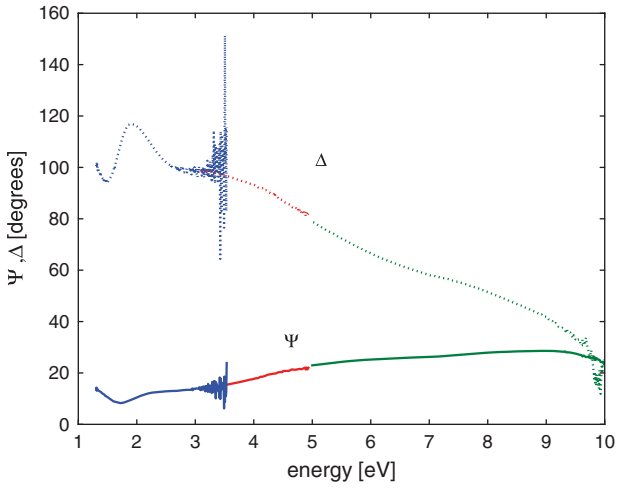

Fig. 1. Three overlapping ellipsometric measurements of a multi-layered sample: visible and near-ultraviolet ranges were studied with a desktop ellipsometer equipped with Avantes light source and CCD detector. The data above 5 eV were obtained using the synchrotron source of BESSY-II.

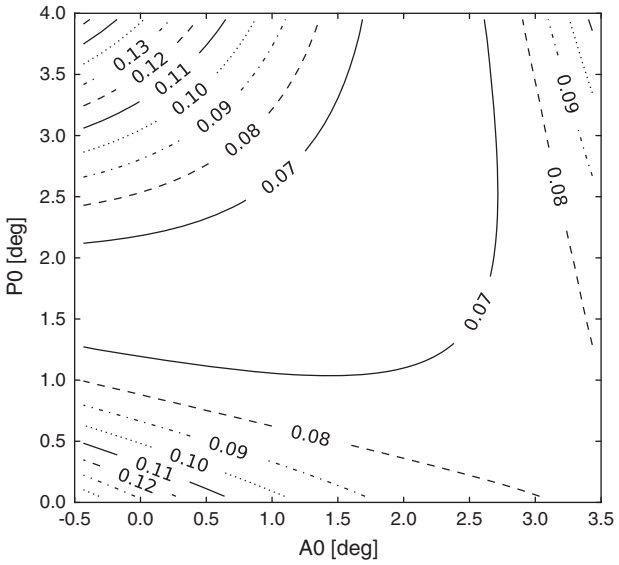

Fig. 2. Map of the absolute error in reconstructed Ψ (average over the whole spectrum) depending on the distance of our estimates of A_0 and P_0 from the true values in the center. The calibration and reconstruction have been done using data from a polarizer setting of $\pm 30°$.

A_0 or P_0 and the true values used in the simulation, on the P_0 values entering the simulation. We used values up to $P_0 = 10°$ while the initial values of the calibration adjustment were assuming a perfect alignment; it means zero starting values for both P_0 and A_0 for the fitting (no a-priori knowledge of the offset). For polarizer settings of $\pm 10°$ and $\pm 20°$ large offsets introduce a strong asymmetry and the fitting procedure often failed to find the right solution with a noise of 0.5% and spectral samples having 500 bins. In Fig. 4 we show only pairs with larger polarizer angles. Nevertheless, the combination of the measurements taken at different polarizer angles gives clearly better results, not only due to the effect of a larger number of spectral points.

When changing A_0 instead of P_0, the mean errors of reconstructed zero angles were almost constant: the average errors of A_0 lie between 0.011° and 0.018° for individual pairs, while they are smaller (0.007°) for the combined calibration. For P_0 the errors in the case of the individual

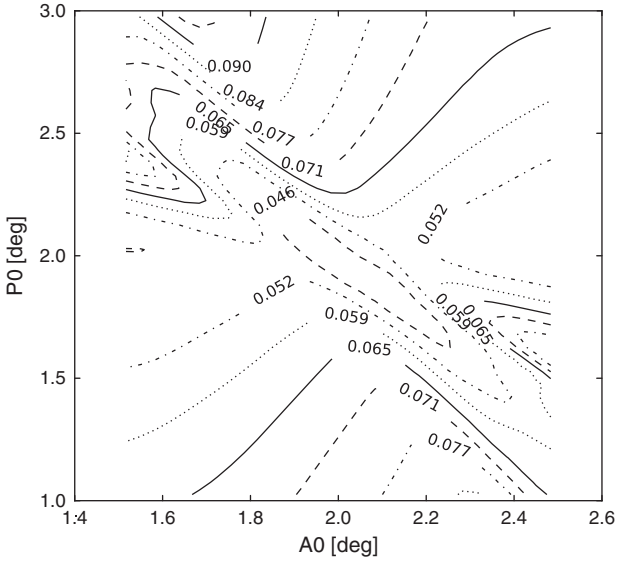

Fig. 3. The same map as in Fig. 2, using data from all 8 polarizer settings, with the minimization of a robust sum described in the text. Note that the map covers a much smaller area compared to Fig. 2.

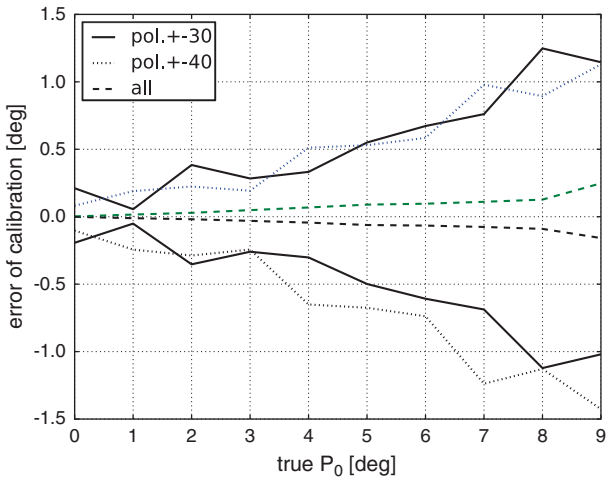

Fig. 4. Errors of reconstructed A_0 (positive values) and P_0 (negative values) as a function of the polarizer misalignment.

pairs lie between 0.005° and 0.015° (depending on the polarizer setting) and they decrease to 0.004° when using the combined dataset.

The choice of the initial range of polarizer settings still plays some role in this process, compared to the method described in [5], where the whole quadrant of polarizer settings is measured. Our approach was motivated by a rather slow movement of polarizing elements with a reasonable exposure time at each position to acquire the whole spectra with a good signal to noise ratio. In ref. [5] the corrections P_0 and A_0 are obtained independently for each spectral point; however, we are looking for a single pair of values for the whole spectrum.

7. Reconstruction errors

Another effect we try to estimate is the influence of input spectra (i.e. the average values of ellipsometric angles) on the errors of reconstructed ellipsometric values. As shown in Fig. 5, we have changed the mean Ψ values in the simulated spectra from 2 to 38°. We have confirmed the expectation that the polarizer azimuth close to the expected Ψ yields the best results. The combined calibration results in a rather flat response, almost everywhere better than the "adapted" polarizer setting.

Undertaking more extensive tests we have calculated the errors of Ψ and Δ for a grid of flat synthetic spectra with the ellipsometric angles ranging from 5° to 40° in Ψ and 0° to 70° in Δ. While the value

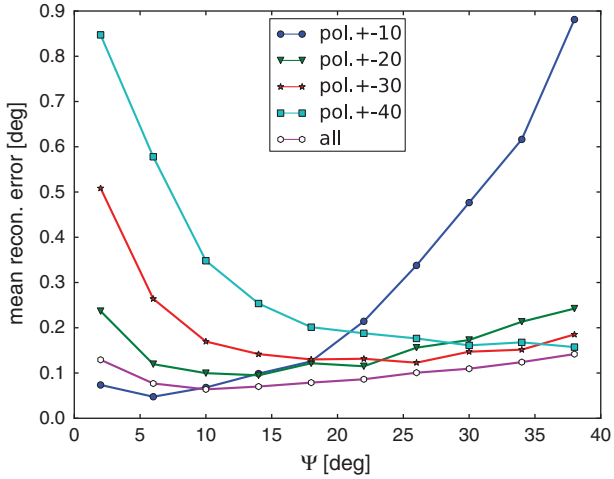

Fig. 5. Difference of the input and the reconstructed Ψ as a function of the initial Ψ and polarizer settings.

of Δ had little effect on the error of reconstructed Ψ, small values of Δ cause large errors in the Δ reconstruction. The dependence of these errors of Δ on Ψ was similar to that shown in Fig. 5.

8. Conclusions

We have found that the calibration procedure based on the measurements at several settings of a polarizer angle provides typically better estimates of the polarizer and analyzer misalignment compared to the calibration as a dedicated process; in addition the latter can be quite time-consuming in the case of FT-IR technique or CCD-based spectroscopy. Our calibration procedure needs no extra experimental time, using measurements at symmetrical settings of the fixed polarizing element both for the extraction of ellipsometric angles and the estimation of offsets of the polarizer and analyzer positions.

Another difficulty with the standard single-energy calibration can be the choice of a suitable photon energy where the procedure yields the best results. Especially with layered samples that exhibit interferences, finding the right spectral position where the residual function has a parabolic shape requires a highly qualified guess.

Numerical studies have confirmed that our calibration procedure proves to be robust and less sensitive to the misalignment of both polarizer and analyzer zero positions if we use several pairs of polarizer settings instead of a single pair of measurements. Since the reconstruction power for a given pair of polarizer settings depends on the true Ψ and Δ values of the sample (the optimal performance occurs when the polarizer angle matches the value of Ψ), using combinations of different polarizer settings seems to be the best approach for samples with strongly variable optical response.

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